

Additional file 2: Derivation of the termination criterion CM

The relative error in the solution \mathbf{x} at the i -th iteration of the PCG method is defined as:

$$e_{r,i} = \frac{\|\mathbf{x} - \hat{\mathbf{x}}_i\|}{\|\mathbf{x}\|} \quad (1)$$

where $\hat{\mathbf{x}}_i$ is an approximate solution of \mathbf{x} at the i -th iteration and $\|\cdot\|$ is the 2-norm.

The preconditioned system of linear equations has the form:

$$\tilde{\mathbf{M}}^{-1}\mathbf{C}\mathbf{x} = \tilde{\mathbf{M}}^{-1}\mathbf{b}$$

where \mathbf{C} is a symmetric (semi-)definite coefficient matrix, \mathbf{b} is the right-hand side, and $\tilde{\mathbf{M}}$ is a preconditioner.

Using the fact that $\|\tilde{\mathbf{M}}^{-1}\mathbf{b}\| = \|\tilde{\mathbf{M}}^{-1}\mathbf{C}\mathbf{x}\| \leq \|\tilde{\mathbf{M}}^{-1}\mathbf{C}\|\|\mathbf{x}\|$, it follows that:

$$\begin{aligned} e_{r,i} &= \frac{\|\mathbf{x} - \hat{\mathbf{x}}_i\|}{\|\mathbf{x}\|} \\ &= \frac{\|\mathbf{C}^{-1}(\mathbf{b} - \mathbf{C}\hat{\mathbf{x}}_i)\|}{\|\mathbf{x}\|} \\ &= \frac{\|\mathbf{C}^{-1}\tilde{\mathbf{M}}\tilde{\mathbf{M}}^{-1}\mathbf{r}_i\|}{\|\mathbf{x}\|} \\ &\leq \frac{\|(\tilde{\mathbf{M}}^{-1}\mathbf{C})^{-1}\|\|\tilde{\mathbf{M}}^{-1}\mathbf{r}_i\|}{\|\mathbf{x}\|} \\ &\leq \|\tilde{\mathbf{M}}^{-1}\mathbf{C}\| \|(\tilde{\mathbf{M}}^{-1}\mathbf{C})^{-1}\| \frac{\|\tilde{\mathbf{M}}^{-1}\mathbf{r}_i\|}{\|\tilde{\mathbf{M}}^{-1}\mathbf{b}\|} \\ &\leq \kappa(\tilde{\mathbf{M}}^{-1}\mathbf{C}) \frac{\|\tilde{\mathbf{M}}^{-1}\mathbf{r}_i\|}{\|\tilde{\mathbf{M}}^{-1}\mathbf{b}\|} \end{aligned}$$

where $\kappa(\tilde{\mathbf{M}}^{-1}\mathbf{C}) = \|\tilde{\mathbf{M}}^{-1}\mathbf{C}\| \|(\tilde{\mathbf{M}}^{-1}\mathbf{C})^{-1}\|$ is the effective spectral condition number of $\tilde{\mathbf{M}}^{-1}\mathbf{C}$.